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Acro User Manual

Version 1.0

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Abstract This document provides a user's guide for the Acro software library. The Acro Project is an effort to facilitate the design, development, integration and support of optimization software libraries. The goal of the Acro Project is to develop (parallel) optimization solvers and libraries using object-oriented software frameworks that facilitate the application of these solvers to large-scale engineering and scientific applications. Thus Acro includes both individual optimization solvers as well as optimization frameworks that provide abstract interfaces for flexible interoperability of solver components. Acro has been written to support optimizers that are broadly useful for DOE's engineering and scientific applications. In particular, many solvers included in Acro can exploit parallel computing resources to solve optimization problems more quickly.

acro - From Greek akros, at the point, end, or top.

acro - A generic term for warblers of the genus *Acrocephalus*, usually referring to the sedge and/or reed warblers. The sedge warbler is a small, quite plump, warbler with a striking broad creamy stripe above its eye, and greyish brown legs. It is brown above with blackish streaks and creamy white underneath. It spends summers in the UK and winters in Africa, south of the Sahara Desert. Its song is a noisy, rambling warble compared to the more rhythmic song of the reed warbler.

acro - A Common Repository for Optimizers

1 Introduction

This document provides a user’s guide for the Acro software library. The Acro Project is an effort to facilitate the design, development, integration and support of optimization software libraries. The goal of the Acro Project is to develop (parallel) optimization solvers and libraries using object-oriented software frameworks that facilitate the application of these solvers to large-scale engineering and scientific applications. Thus Acro includes both individual optimization solvers as well as optimization frameworks that provide abstract interfaces for flexible interoperability of solver components. The optimization packages in Acro have been written to support optimizers that are broadly useful for DOE’s engineering and scientific applications. In particular, many solvers included in Acro can exploit parallel computing resources to solve optimization problems more quickly.

The Acro framework uses a two level software structure that connects a system of *packages*. An Acro package is usually developed by a (relatively) small set of developers to solve a specific set of problems. Packages exist beneath the Acro top level, which provides a common look-and-feel. Each package has its own structure, documentation and set of examples, and it is possibly available independently of Acro. However, Acro provides a framework for exploiting synergy between packages in a flexible manner.

Acro currently includes about ten different packages, several of which include interfaces to external software libraries. The entire set of packages covers a variety of algorithmic and numerical methods for optimization, as well as utilities that facilitate the development of software for scientific computing. A detailed description of each Acro package is beyond the scope of this document. Instead, we provide a birds-eye view of the Acro packages and their corresponding solvers. We also include information about how Acro can be installed and used. Further, we provide pointers to additional package documentation.

2 Software Overview

Acro integrates a variety of optimization software packages, including libraries developed at Sandia National Laboratories as well as publicly available third-party libraries. The goal of this integration is to provide a single framework that includes a wide range of optimization methods.

2.1 Capabilities

Three classes of optimizers are well-represented in Acro:

1. branch-and-bound methods for integer programming
2. heuristic global optimization methods
3. derivative free local optimization methods

2.1.0.1 Integer Programming The **PICO** package defines an object-oriented scalable library for branch-and-bound. In particular, **PICO** includes a well-developed parallel mixed integer linear programming (MILP) solver. **PICO** depends on **UTILIB** for many basic data structures and

system utilities. Additionally, **PICO** uses the **COIN** interface library to encapsulate linear programming solvers. Two publicly available linear programming solvers are integrated into Acro: **SOPLEX** and **CLP** (which is included in **COIN**). The **mpPCx** parallel linear programming solver is also being developed at Sandia (this is currently not part of Acro).

PICO has been integrated with the **GLPK** package to support a public domain interface to AMPL integer programming problems. **PICO** has also been integrated with the **AMPL** package, which includes the AMPL routines for setting up an AMPL solver.

2.1.0.2 Global Optimization The **COLIN** package defines a general-purpose interface for optimization solvers. Although many C++ optimization software libraries have been developed, these designs invariably incorporate specific features that facilitate the development and application of the author's algorithms. By contrast, COLIN is intended to provide a generic interface for optimizers that is simple to use and which can encapsulate the basic algorithmic interface of a wide range of general-purpose optimizers. As such, COLIN can be used as 'middle-ware' to facilitate the interface of an optimizer to (a) other optimizers to form hybrid solution strategies and (b) to generic user-interfaces like AMPL or Excel, for which well-defined APIs exist.

The **Coliny** package defines a variety optimizers using COLIN. In particular, **Coliny** includes global optimization heuristics like multi-start local search, evolutionary algorithms and DIRECT. Additionally, **Coliny** includes COLIN interfaces to several other global optimization solvers, including a Lipschitzian solver defined using **PICO**. The **3po** package includes COLIN interfaces for a variety of other publicly available optimizers.

2.1.0.3 Derivative Free Optimization Derivative free optimizers perform local optimization on continuous search domains without the aid of gradients or other derivative information. The **Coliny** solver includes several derivative free methods, and in particular a variety of pattern search methods. The **APPSPACK** package defines a parallel pattern search method that exploits a novel asynchronous parallel search.

2.2 End-User Applications

The principal goal of Acro is to provide support of optimization libraries. However, there are several end-user applications that can be build within Acro.

1. **PICO** - a solver for mixed-integer linear programming problems. **PICO** can be use with AMPL, or with user-input files in standard formats (LP, MPS, etc).
2. **coliny** - a solver for derivative-free and heuristic global optimization. **coliny** is principally indended for use with AMPL.

Documentation for the use of these solvers is currently being developed.

2.3 Overview of Acro Packages

Acro is organized around a set of closely related software packages. Figure 1 illustrates the dependencies between these packages; the dashed lines indicate packages and dependencies that are currently being developed.

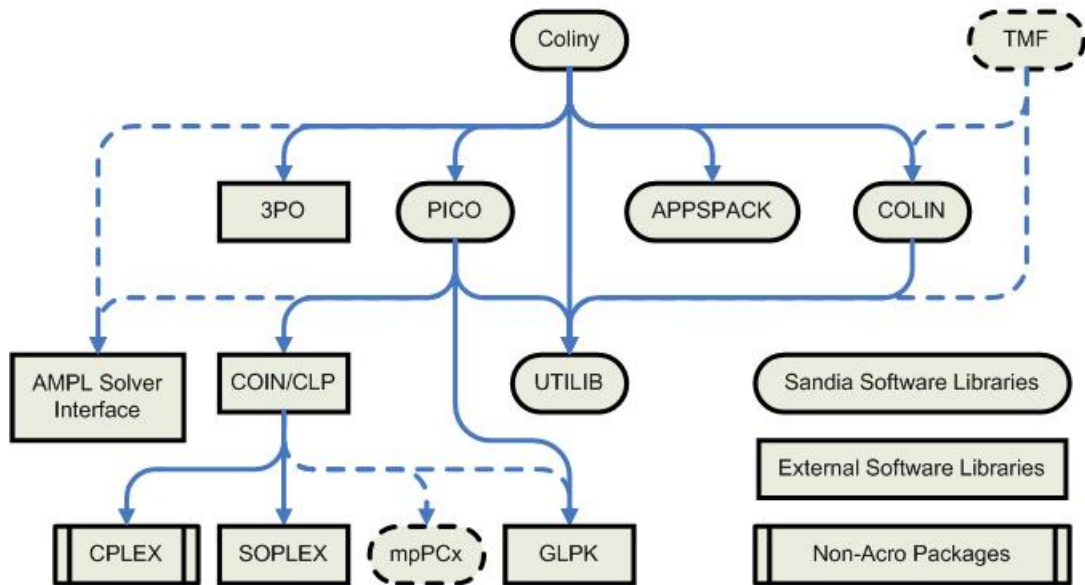


Figure 1: An illustration of inter-package dependencies within Acro.

1. **3po** - A library of third party optimizers that are publicly available.
2. **CMO** - An example of the use of the MW software for parallel master-worker. This is not a core Acro package, and thus it will be reconstituted shortly.
3. **COIN** - A subset of the COIN optimization repository that includes linear and integer programming interfaces for a variety of third-party software projects. This package uses the Acro configure/makefile's, since COIN does not have a sufficiently flexible configure/build process. See <http://www.coin-or.org> for further information on this software.
4. **SOPLEX** - The SOPLEX linear programming library. SOPLEX contains an implementation of the revised simplex algorithm. It features primal and dual solving routines for linear programs and is implemented as a C++ class library that can be used with other programs. See <http://www.zib.de/Optimization/Software/Soplex/> for further information on this software.
5. **ampl** - This package includes C files provided by AMPL to setup solvers that can be used by AMPL. In particular, this package provides the ability to read the AMPL *.nl file format.
6. **appspack** - An asynchronous parallel pattern search method developed at Sandia National Laboratories. See <http://software.sandia.gov/appspack/> for further information on this software.
7. **colin** - A general-purpose C++ optimization interface developed at Sandia National Laboratories. This library provides a middle-ware layer for optimizers that facilitates the use of hybrid optimizers, as well as optimizers applied to novel, user-defined search domains.
8. **coliny** - Coliny is a collection of C++ optimizers that are derived directly from the COLIN interface. This library includes methods such as pattern search, evolutionary algorithms,

multistart local search and DIRECT. Coliny is a revision of the older SGOPT library, which is now deprecated.

9. **glpk** - The GNU linear programming toolkit. GLPK is intended for solving large-scale linear programming (LP), mixed integer programming (MIP), and other related problems. See <http://www.gnu.org/software/glpk/glpk.html> for further information on this software.
10. **pico** - PICO defines a flexible branch-and-bound engine that uses an object-oriented model to allow it to be easily adapted to new applications. A novel feature of PICO is its ability to scale up parallel branch-and-bound to thousands of processors. PICO also includes solvers for mixed-integer linear programming.
11. **sgopt** - SGOPT defines a collection of C++ optimizers. This software has been superceded by Coliny, and its use is now deprecated.
12. **tmf** - TMF is a Templatized Metaheuristics Framework that is under development.
13. **utilib** - UTILIB is a library of C and C++ utility methods. It includes classes of standard data structures, general-purpose mathematical routines, sorting methods, random number generators, tools for processing command-line options and tools to support parallelization of software.

3 Software Management

3.1 Downloading

The Acro software can be downloaded as a compressed tarfile from <http://software.sandia.gov/Acro/>.

Alternatively, Acro can be checked out from the Acro CVS (Concurrent Version System) repository. The CVS repository for Acro can be accessed by executing

```
cvs -d :ext:${userid}@software.sandia.gov:/space/CVS-Acro checkout acro
```

This requires the use of an account (userid) on **software.sandia.gov**. Accounts on this machine are generally restricted to Sandians and academic collaborators working with Sandians. The scripts **cvs.a** and **ssh.cvs** can be used to encapsulate the access to this repository in a convenient manner; these scripts can be downloaded from <ftp://ftp.cs.sandia.gov/pub/papers/wehart/src/shells>.

By default, the **cvs.a** script uses the unix command **whoami** to determine the user id for the cvs connection. In general, the id `${userid}` on `software.sandia.gov` will be selected by Sandia administrators. If this does not match your id provided by **whoami**, then you can set the **ACRO_USER** environmental variable to be id on `software.sandia.gov`. For example, within a `csh` environment, you would do

```
setenv ACRO_USER janedoe
cvs.a checkout acro
```

to checkout Acro from the account `janedoe@software.sandia.gov`.

The Acro CVS repository is organized into different modules that include different subsets of the Acro packages:

- **acro** - The Acro repository with all software packages and an integrated configuration facility that builds them
- **acro-coliny** - The Acro repository with the Coliny software package and all packages that it depends on
- **acro-pico** - The Acro repository with the PICO software package and all packages that it depends on

3.2 Online Resources

The CVS repository for Acro is on `software.sandia.gov`. This machine supports a variety of tools to facilitate the development of software tools, including

1. Bugzilla (<http://software.sandia.gov/bugzilla/>) - online bug reporting
2. Mailman (<http://software.sandia.gov/mailman/listinfo/>) - mailing list management
3. Bonsai (<http://software.sandia.gov/bonsai/cvsqueryform.cgi>) - a query interface to CVS

The following mailing lists are supported for Acro:

1. `acro-announce@software.sandia.gov` - general announcements
2. `acro-bugs@software.sandia.gov` - bug reports
3. `acro-checkins@software.sandia.gov` - CVS checking reports
4. `acro-developers@software.sandia.gov` - a developers mailing list
5. `acro-help@software.sandia.gov` - a help list
6. `acro-misc-checkins@software.sandia.gov` - CVS checking reports for miscellaneous acro components
7. `acro-users@software.sandia.gov` - a general users' mailing list

The mailman server also includes some mailing lists for specific Acro components like APPSPACK, PICO and Coliny.

4 Installation

4.1 Standard UNIX Installation

After the Acro software has been downloaded, it must be configured for building on specific hosts for specific target platforms. Installation on UNIX systems is performed by the following steps:

1. If you have an archive, unpack it as follows

```
gunzip acro-$VERSION.tar.gz    # uncompress the archive
tar xf acro-$VERSION.tar       # unpack it
```

2. Move into the **acro** directory and run the **configure** script.

```
cd acro
./configure
make
```

This will configure the software for your machine and compile the Acro library (see Section **Configuration** (p.12) for more details concerning configuration options and the details of the configuration process). After building Acro, the Makefile scripts will create links to package header directories in the directory **acro/include**, and links to all package libraries are included in **acro/lib**. Note that the makefiles in Acro may not be portable to all **make** commands. However, they do work with the GNU **gmake** command.

You can remove object files, libraries, and executables by typing

```
make clean
```

If you wish to re-configure your Acro source from scratch or re-generate all custom makefiles, type

```
make distclean
```

This will remove all symbolic links, custom makefiles, and **config.status** files. This will require a re-configure of the system and is usually done in preparation for updating source in the CVS repository or creating tape archives for distribution.

4.2 Custom UNIX Installation

Acro can also be built with the following custom configure/build process

```
cd acro
./setup configure build
```

This custom configure/build process overcomes a common problem with the standard configure/build process: it can create a voluminous output that is difficult to follow and which can mask the fact that there errors have occurred. This is a particular issue for large projects like Acro, which has many independent packages that may fail to configure or build.

The **setup** command performs the following actions

-
1. Pipe the configuration output into `acro/test/config.out` and generate a `test/config.xml` summary file
 2. Pipe the build output into `acro/test/build.out` and generate a `test/build.xml` summary file (this includes builds of Acro executables and test executables)

The XML files generated in the `acro/test` director provide a quick reference to confirm that the software was configured and built properly. The use of **setup** can be extended to include configuration options, and to perform tests. For example the following configures using MPI and performs fast smoke tests of various Acro packages:

```
cd acro
./setup configure --with-mpi build smoke
```

4.3 Setup Documentation

The main Acro makefile includes several targets for generating documentation. This documentation is generated with the **doxygen** utility, so documentation can be generated in several formats. The command

```
make html
```

creates HTML documentation, and the command

```
make pdf
```

creates documentation in a single PDF file. This later command requires the use of **latex**, **dvips** and **ghostscript** packages.

5 Acro Licenses

The Acro framework is licensed with the GNU lesser general public license (see below). Acro includes a variety of third-party software packages, which have separate licensing policies. These licenses are included here to provide a single point of reference for the use of Acro. The following list describes the licenses for the different Acro packages:

1. UTILIB, PICO, SGOPT, Coliny, COLIN, APPSPACK, glpk
The GNU Lesser General Public License (p. 24)
academic, commercial
2. Any.h (utilib/src/adt)
BOOST License (p. 16)
academic, commercial

-
3. RANLIB (utilib/src/ranlib)
RANLIB License (p. 16)
academic, commercial
 4. COIN and CLP
Common Public License (p. 17)
academic, commercial
 5. Soplex
ZIB Academic License (p. 21)
academic
 6. ampl
Lucent Technologies License (p. 23)
academic, commercial

These licenses are provided in Appendix **Licensing Details** (p. 16) generally allow for unrestricted academic use. The Soplex license is restricted to academic users, but the CLP linear programming license is available for commercial use.

Please contact the original software developers if you have questions concerning the use of these software components. Further, you can contact acro-help@software.sandia.gov for assistance if you decide that you wish to build Acro without some particular software component.

6 References

The following are sources of package-specific documentation that provide more detail on the use of Acro.

1. W. E. Hart. UTILIB user manual version 1.0. Technical Report SAND2001-3788, Sandia National Laboratories, 2001.

7 Acknowledgements

The Acro Project grew out of the ongoing development of the UTILIB, SGOPT, Coliny, and PICO libraries within the Discrete Algorithms and Mathematics Department. In particular, the development of PICO and Coliny increasingly required the integration of third-party libraries. Although a variety of people have contributed to the Acro packages, I would like to thank Cindy Phillips, Jonathan Eckstein, Mario Alleva, Shannon Brown and Mike Eldred for their input on these software libraries, which ultimately influenced the design of Acro itself. The design of Acro has been significantly influenced by their feedback.

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We are grateful to Mike Langman for graciously allowing us to use his beautiful Sedge Warbler illustration. Other illustrations and photographs by Mike Langman are available at [Mike Langman Bird Art](#).

A Configuration

A.1 Overview

The **configure** script automates much of the setup activity associated with building large suites of programs like Acro on various hardware platforms. This includes

1. making symbolic links so that files used for configuration can be accessed from one location
2. generating Makefiles so that objects, libraries, executables and other 'targets' can be created for specific and unique hardware platforms
3. calling itself recursively so that sub-directories can also be configured

There are a number of configuration options that can be used to customize the installation. The core parameter list for the **configure** script is:

```
configure hosttype [--target=target] [--srcdir=dir] [--rm]
                  [--site=site] [--prefix=dir] [--exec-prefix=dir]
                  [--program-prefix=string] [--tmpdir=dir]
                  [--with-package[=yes/no]] [--without-package]
                  [--enable-feature[=yes/no]] [--disable-feature]
                  [--norecursion] [--nfp] [-s] [-v] [-V | --version]
                  [--help]
```

Many of these options are not necessary since system information can be often acquired from your local machine. Refer to the Cygnus **configure** documentation for complete information.

A.2 Standard Options

The following options are either commonly used or specific to Acro packages:

<code>[-with-compiler=<gcc,CC>]</code>	Sets up a specific compiler; The native compiler is the default.
<code>[-target=<solaris>]</code>	Optional flag to specify the target machine that you are cross-compiling for.
<code>[-site=<snl980>]</code>	Specifies the site-specific locations for MPI, etc.
<code>[-with-debugging]</code>	Turns on the DEBUGGING macro and sets the OPTIMIZATION macro to <flag> (code is compiled with -g by default).
<code>[-with-mpi]</code>	Turns on the use of the MPI package.
<code>[-with-mpe]</code>	Turns on the use of the MPE package.
<code>[-with-swig]</code>	Enables the use of swig to wrap Acro packages for use with the Python scripting language.
<code>[-with-static]</code>	Enables the compilation of statically linked libraries (the default).
<code>[-with-insure]</code>	Enables the compilation with the insure++ debugging tool.
<code>[-with-shared]</code>	Enables the compilation of dynamically linked libraries, which can be shared.
<code>[-with-optimization=<level>]</code>	Sets the optimization level used when compiling the source files. This is overridden by the <code>-with-debugging</code> flag.
<code>[-with-gprof]</code>	Sets the compiler to use flags that force executables to dump output files that can be read by the unix gprof utility to profile the code.

A.3 Details of the Configuration Process

The **configure** script creates Makefiles from **Makefile.in** template files, which outline the basic ‘targets’ that need to get built. This script can be customized using the **configure.in** file. Variables that are package, site or hardware dependent are stored in individual ‘fragment’ files. These ‘fragment’ files are added to the custom created Makefiles using the host, target, package and/or site parameters. After the **configure** command is completed, three files will be generated in each configured directory.

1. Makefile-`{target}`

The suffix, `{target}`, will depend on the target architecture, which defaults to the host architecture; native builds have identical host and target values.

2. Makefile

This will be a symbolic link to **Makefile-`{target}`**. Consequently, when **make** is executed, the default behavior is to use the last generated Makefile-`{target}` file.

3. config.status

A ‘recording’ of the configuration process (i.e., what configure options were used to generate the current makefile).

Running **configure** takes a while, so be patient. Verbose output will always be displayed unless the parameter ‘`-silent`’ is used. Further, the parameter ‘`-norecursion`’ can be used to configure only the current directory. All generated **config.status** files include this parameter as a default for easy makefile re-generation; after editing a **Makefile.in** file, you can construct the associate Makefile file by executing **config.status**.

The **configure** command supports multi-platform environments using Makefile fragment files. The fragment files for these platforms and for the packages that Acro relies on are located in the **acro/config** directory. There are five types of files in this directory:

```
mh-<host>
Fragments that define the utilities provided by the host (e.g. the
definition of MAKE).

mp-<target>-<site>
Fragments that define information for the packages that are used by
Acro (e.g. MPI).

ms-<site>
Fragments that define the site-specific general configuration
information. If this does not exist for a given site, then the
default ms-default fragment is used.

mt-<target>
Fragments needed to specify how to compile code for a target
architecture (e.g. compiler name/location).

mf-<host>-<target>-<site>
Automatically generated by the configure scripts.
```

A.4 Platforms Supported

Acro can be configured for code development and execution on the following platforms:

SUN	Solaris 2.8	CC v5.4	solaris
PC	Red Hat LINUX 9	g++ v3.2.2	linux
SGI	IRIX 6.5	CC v7.41	irix
DEC	OSF 5.1	cxx v6.3-002	osf
IBM	AIX 5.1	x1C v6	aix
TFLOP	Cougar (compute)	ciCC v4.4.0	cougar

TFLOP	OS (service)	iCC v4.4.0	tflop
Cplant	Compute OS	c++	cplant
Cplant	Service OS	g++	cplant
PC	Windows (Cygwin)	g++	cygwin
Mac	OSX (Darwin)	g++	darwin
HP	HP-UX 10.20	CC	hpux

The last column shows the configuration target used to configure Makefiles for each of these systems.

The standard configure and build process described in Section **Installation** (p.8) works on almost all of these platforms. A notable exception are cougar builds, which generate executables for the ASCI Red compute nodes. These builds need to be performed with a cross-compiler. For example, when building on `sasn100.sandia.gov`, you would configure as follows:

```
./configure --site=sasn100 --target=cougar
```

B Licensing Details

Acro includes a variety of third-party software packages, which have separate licensing policies. These licenses are included here to provide a single point of reference for the use of Acro. These licenses generally allow for unrestricted academic use. The SOPLEX license is restricted to academic users, but the CLP linear programming license is available for commercial use.

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```
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//
// Permission to use, copy, modify, and distribute this software for any
// purpose is hereby granted without fee, provided that this copyright and
// permissions notice appear in all copies and derivatives.
//
// This software is provided "as is" without express or implied warranty.
```

B.2 RANLIB License

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Krogh, F. Algorithms Policy. ACM Tran. Math. Softw. 13(1987), 183-186.

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